SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CA18222
STSM title: Charge Migration Encoded in Quantumpath Interferometry of Molecular System
STSM start and end date: 12/10/2020 to 30/10/2020
Grantee name: Leena Abusin

PURPOSE OF THE STSM:

(max.200 words)
In order to retrieve ultrafast dynamical information of charge migration in molecular systems, pumpprobe measurements employing femtosecond to attosecond pulses are needed. These pump-probe approaches unable us to access electronic and nuclear dynamics after ionisation of molecules subject to ultrafast laser fields. It is fundamentally important to understand these first instants of cationic dynamics as they are of complex nature. They bear correlated electronic and nuclear quantum dynamics that trigger chemical properties of the molecular systems. Ultimately, this will lead to quantum control of molecular properties and to understanding chemical processes involved in light harvesting and catalysis. There are two strategies to employ ultra-fast pump-probe schemes basedon high harmonic generation (HHG) sources: 'ex-situ' and 'in-situ' pump-probe approaches. The ex-situ consists in using an attosecond XUV pulse produced by HHG, often combined either as XUV-IR, XUV-XUV or XUV-VUV. The attosecond time-domain and the in-situ approach analyses the HHG signal itself to access information on the generating medium, with combined attosecond and Ångström resolutions. My task is as a theoretician is to develop and understand Low-Dimensional Models which employ the time-dependant-schrodinger-equation (TDSE) which in turn can be coupled with experimental data. Such an approach is employed in the code MOLBIT developed by Jeremie Cailat and Richard Taieb, it can provide a qualitative description of the dynamics of complex molecules by tracking the time evolution of the wavefunction. Thus learning and applying low-dimensional models will allow me to give insight into the tranision states behind experimental spectroscopic results.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

(max.500 words)
My first task was to understand from a fundamental level, the theoretical reasoning behind the Low-Dimensional Models I would be implementing. The TDSE allows for the propagation of the wavefunction in time. However exact analytical solutions of the TDSE become impossible achieve beyond monoatomic and monoelectronic systems. Computers are not sophisticated enough for calculation of the TDSE for a multielectronic or a multiatomic system. More importantly should the TDSE be solved analytically, the data extracted from multi-electron wavefunctions would not provide any clear information about the physical processes in different stages of the investigative mechanism. Therefore the low-dimensional models I would be using provide a numerical approach to the solution of the wavefunction by descritising the time and space variables and the wavefunction is accessed by solving linear equations. Thus the TDSE is written in the form of the time-evolution wavefunction and we proceed by using a finite difference approximation of that equation. This leads to the crank-nicholson scheme by taking the first order taylor-expansion of the

exponential function. Time and space variables are then dicretised by expressing the differential equations in the Hamiltonian as such. Finally a guass elimination method in used to make unknown variables in the final expression known and ready for computer implantation.
Time was spent learning the basics of the language Fortran90 in order to implement the code myself. Once I become farmilar with the language the final week was dedicated to the practical implantation of a 1-D model where the TDSE is based on a H2+ ion. In my final week I also spent time learning about the MOLBIT code which is a 2-diemsional extention of the 1-D model by expressing electron-nuclear correlations.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

I developed a code that describes the time-propagation of the electronic wavepacket in a diatomic hydrogen ion. I learned and understood the MOLBIT code which I can use to compute the dipole acceleration of the electron which will correlate to experimental HHG data that is worked on within my group. The foremost objective of this mission was to learn and in doing so I have a strong understanding of low-dimensional models and their implemtation using the Fortran language.

FUTURE COLLABORATIONS (if applicable)

It has been planned that we keep in contact by making use of online forums. In terms of meeting with the collaborators face-to-face again, nothing has been formally declared as of yet.